

# The Role of Chaos in One-Dimensional Heat Conductivity

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We investigate the heat conduction in a quasi 1-D gas model with various degree of chaos. Our calculations indicate that the heat conductivity  $\kappa$  is independent of system size when the chaos of the channel is strong enough. The different diffusion behaviors for the cases of chaotic and non-chaotic channels are also studied. The numerical results of divergent exponent  $\alpha$  of heat conduction and diffusion exponent  $\beta$  are in consistent with the formula  $\alpha = 2 - 2/\beta$ . We explore the temperature profiles numerically and analytically, which show that the temperature jump is primarily attributed to superdiffusion for both non-chaotic and chaotic cases, and for the latter case of superdiffusion the finite-size affects the value of  $\beta$  remarkably.

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## I. INTRODUCTION

The low dimensional microscopic dynamics of heat conduction has been an attractive question since early year last century. Much more attention has been payed to this problem in the last two decades due to the dramatic achievement in the application of miniaturized devices [1, 2, 3, 4, 5, 6] which can be described by 1D or 2D models. More and more numerical calculations are focused on the minimal requirements for a dynamical model where Fourier's law holds or not [7, 8, 9, 10, 11, 12, 13, 14, 15, 16]. A convergent heat conductivity was shown in ding-a-ling model [8, 9] which is chaotic. The studies on Lorentz gas model [10, 11] (the circular scatters are periodically placed in the channel) of which the Lyapunov exponent is nonzero gave a finite heat conductivity which fulfils the Fourier law explicitly. Hence, chaos was ever regarded as an indispensable factor to normal heat conduction. Whereas, the FPU model [12, 13] indicated that the chaotic behavior is not sufficient to arrive at normal heat conduction. Recently, a series of billiard gas models [10, 14, 15, 16] were devoted to explore the normal heat conduction of quasi 1D channels with zero Lyapunov exponent. However, the role of chaos in heat conduction has not been well understood. Additionally, the exponential stability and instability frequently coexist in the scatters of real system. Thus the model with various degree of chaos deserves further investigation from the microscopic point of view, and it will be also interesting to explore non-equilibrium stationary states and to determine the steady temperature field.

In this paper, we focus on the quasi one-dimensional gas model which is closer to the real system. The scatters in our model are the isosceles right triangle with a segment of circle substituting for the right angle. In this case the edges of scatters are the combination of line and a quarter of circle. Such a channel is of chaos, which indicates exponential instability of microscopic dynamics. Our paper is organized as follows. In section II, we introduce the model and investigate the degree of chaos for various channels with different arc-radius and channel

height. In section III, we study the heat transport behavior and the corresponding diffusive behavior by changing the radius of top arc and channel height. In section IV, we investigate the non-equilibrium stationary state and determine the steady temperature field numerically. We also analyze the dependence on diffusion exponent  $\beta$  and system size  $N$  of temperature profile theoretically. In section V, we discuss the relation between our work and others and summarize our main conclusions.

## II. THE MODEL

We consider a billiard gas channel with two parallel walls and a series of scatters. The channel consists of  $N$  replicate cells of length  $l$  and height  $h$ , and each cell is placed with two scatters as shown in Fig. 1. The scatter's geometry is an isosceles right triangle of hypotenuse  $a$  whose vertex angle is replaced by a segment of circle with radius  $R$  which is tangential to the two sides of the triangle. At the two ends of the channel are two heat baths with temperature  $T_L$  and  $T_R$ . Noninteracting particles coming from these heat baths are scattered by the walls and the straight lines as well as the arcs of the scatters in the channel.

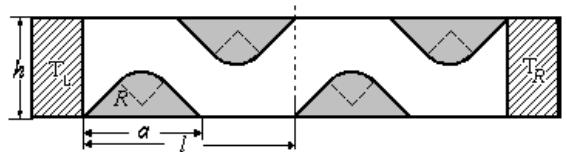


FIG. 1: The channel with  $N$  replicate cells. Here,  $l = 2.2$ ,  $a = 1.2$ ,  $h$  changes from 1.0 to 0.27, and  $R$  from 0 to 0.848528 to ensure a quarter of circle always.

For such a channel, the degree of chaos can be characterized qualitatively by Poincare surface of section (SOS) [17]. Suppose we take out one unit cell from the channel and close the two ends by straight walls. Then the prob-

lem becomes a billiard problem. A particle moves within the cell and makes elastic collision with the mirror-like boundary. We investigate the surfaces of section ( $s, v_\tau$ ) under different initial conditions.  $s$  is the length along the billiard boundary from the collision point to the reference point.  $v_\tau$  is the tangential component of velocity with respect to the boundary at that point. The filling behavior of phase space shown in Fig. 2 indicates the degree of chaos. In case I, it's non chaotic. The surface of section is regular and periodic as shown in Fig. 2(a). As the radius  $R$  is increased from (a) to (e), the motion becomes more complex and the map becomes dense with points except some regular islands. In Fig. 2(f), the regular parts disappear which indicates strong chaos.

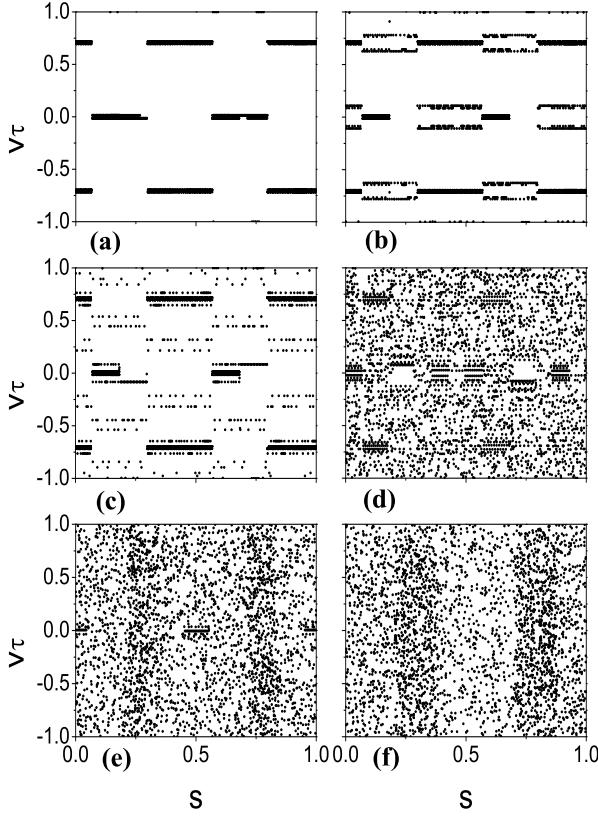


FIG. 2: Poincaré surface-of-section of the billiard problem. The billiard starts with an incident angle 0.8 and unit velocity. (a)  $R = 0, h = 1.0$ ; (b)  $R = 0.001, h = 1.0$ ; (c)  $R = 0.015, h = 1.0$ ; (d)  $R = 0.1, h = 1.0$ ; (e)  $R = 0.848528, h = 1.0$ ; (f)  $R = 0.848528, h = 0.27$ .

### III. THE HEAT TRANSPORT AND DIFFUSION BEHAVIOR

To study the heat conduction of the model, the heat flux is investigated firstly. In calculating the heat flux, we follow Ref. [10]. For simplicity, the particles from the two heat baths are supposed to have definite velocities  $\sqrt{2T_L}$

and  $\sqrt{2T_R}$  respectively [14]. We consider one particle colliding with a heat bath during a period of simulating time. The energy exchange  $(\Delta E)_j$  at the  $j$ th collision with the heat bath is defined as

$$(\Delta E)_j = E_h - E_p, \quad (1)$$

where  $E_h$  denotes for the energy of particle taken from the bath and  $E_p$  for that carried in the channel. For  $M$  collisions between the particle and the bath wall during the simulation time  $t$ , the heat flux is given by

$$J_1(N) = \frac{\sum_{j=1}^M (\Delta E)_j}{t}. \quad (2)$$

As there is one heat carrier in each cell and the channel has  $N$  replicas, there are  $N$  particles in the whole channel. Summing over the heat flux of  $N$  heat carriers, we have  $J_N(N) = NJ_1(N)$ . Meanwhile, the Fourier's law reads

$$J_N(N) = -\kappa \frac{dT}{dx} = \kappa \frac{T_L - T_R}{Nl}, \quad (3)$$

where  $\kappa$  refers to the heat conductivity which is determined by Eqs. (2) and (3),

$$\kappa \sim N^2 J_1(N). \quad (4)$$

We consider various cases by changing the radius  $R$  of the top arc of the scatter to investigate their effects on heat conduction. The heat flux of a single particle versus system size shown in Fig. 3 are four typical cases. Namely, case I: the ■ studies for  $R = 0, h = 1.0$ ; case II: the ◦ for  $R = 0.001, h = 1.0$ ; case III: the △ for  $R = 0.848528, h = 1.0$ , and case IV: the ▽ for  $R = 0.848528, h = 0.27$ , respectively. The total cell numbers are chosen as  $N = 20, 40, 80, 160, 320, 640$  and 1280 respectively. After a sufficient long period of simulation time, the heat flux approaches to a constant value. Clearly, the value of heat flux decreases with increasing  $R$  for the same size. Remarkably, there is 20 times difference of heat flux between case III and case IV, which indicates that smaller height suppresses the heat flux greatly. Thus, it appears that the value of heat flux can be adjusted in this way in designing heat-control devices. Furthermore, our calculations show that the heat flux dependence on  $N$  exhibits faint non-linearity although the curve looks linear for all cases except case IV in the log-log scale.

In order to observe the deviation from the line, which arises from the finite-size effect, we calculate the ratio of heat flux versus system size for various radius. The data for the aforementioned four cases are plotted in the right panel of Fig. 3, from which one can see that both the increasing of system size and of the arc radius bring the ratio an upward tendency to the value 4 which ensures the Fourier law. In case I where  $R = 0$ , there is only a slight increase for the ratio around 2.4. Whereas, the ratio rises drastically along with the increasing of systems

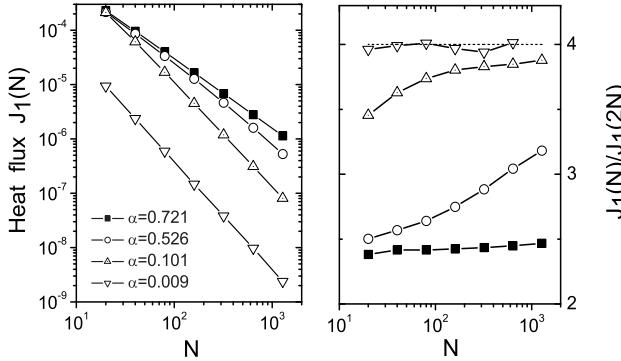


FIG. 3: The heat flux of a single particle versus system size ( $N = 20, 40, 80, 160, 320, 640$  and  $1280$ ) with the divergence exponent of heat conductivity  $\alpha = 0.721, 0.526, 0.101, 0.009$  for four typical cases respectively (left panel). The ratio of heat flux  $J_1(N)/J_1(2N)$  for different system sizes (right panel).

size even if the radius  $R$  is merely  $0.001$  (the case II). When  $R = 0.848528$  (the case III), the scatters become a full segment of quarter circle. The ratio also rises drastically at first and gradually after  $N > 160$  in this case. In both cases II and III, it seemly approaches to distinct asymptotic values which are all different from that for normal conduction. This implies that smaller degree of chaos is insufficient to bring about a normal heat conduction although the increasingly chaotic degree makes the divergent exponent of heat conduction smaller. In case IV, we maintain the scatters at radius  $R = 0.848528$  and reduce the height  $h$  from  $1.0$  to  $0.27$ . In this strongly chaotic case, the ratio fluctuates around the value  $4$  (dotted line) which means that Fourier law is obeyed.

It is known that the normal heat conduction happens when  $\alpha = 0$ , which indicates the heat conductivity is independent of system size, and the anomalous heat conduction corresponds to the case of  $\alpha > 0$ . The heat conductivity  $\kappa$  we calculated can be given by  $\kappa \sim N^\alpha$  with  $\alpha \gtrsim 0$  despite the heat-flux ratio has a different increase in asymptotic value for all cases (except case IV).

We calculate  $\alpha$  at the range of system sizes  $N$  from  $20$  to  $1280$  by averaging over many realizations for various radius  $R$  at fixed channel height  $h = 1.0$ , and the plot of the dependence of  $\alpha$  on  $R$  is shown in Fig. 4(a). One can see that  $\alpha$  descends from  $0.721$  through  $0.526$  to  $0.092$  if  $R$  increases from  $0$  to  $0.848528$  for a fixed height  $h = 1.0$ . Clearly, the  $\alpha$  descends rapidly for small radius (e.g.  $R = 0.001$  in case II) and slowly for larger ones. This illustrates that the appearance of arc on the top of the scatter suppresses the divergent exponent  $\alpha$  drastically. If the channel height  $h$  for fixed  $R = 0.848528$  is changed from  $1.0$  to  $0.27$ , the  $\alpha$  is found to diminish to  $0.009$ . Therefore the  $\kappa$  appears to be independent of system size and the Fourier law holds in this case.

Since the characteristic of heat transport is found being closely related to the diffusion behavior[14, 15, 16,

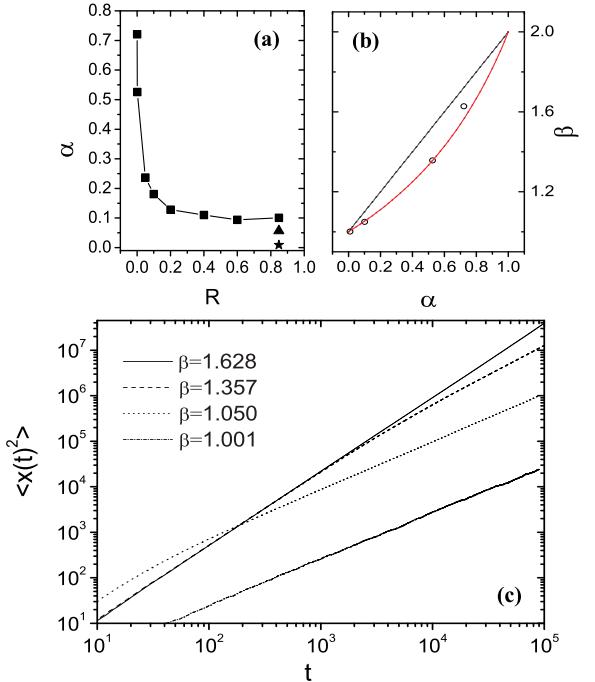


FIG. 4: (color on line) (a) Conductivity divergence exponent  $\alpha$  versus circular radius  $R$ . The ■ refers to the magnitude of  $\alpha$  for  $h = 1.0$ ,  $R = 0, 0.001, 0.05, 0.1, 0.2, 0.4, 0.6$ , and  $0.848528$ ; the ▲ for  $h = 0.5$  and  $R = 0.848528$ ; the ★ for  $h = 0.27$  and  $R = 0.848528$  has the value of  $0.009$ . (b) The relation between  $\beta$  and  $\alpha$ , where the circle is the numerical result, the red line is of  $\alpha = 2 - 2/\beta$  [18] and the dashed line is the result of Ref. [20]. (c) Log-log plot of mean square displacement  $\langle x(t)^2 \rangle$  versus time  $t$ . The curves from top to bottom on the right correspond to cases I, II, III and IV respectively. The ensemble has  $10^5$  particles starting from the center of the channel at time  $t = 0$  where  $x = 0$  with the unit velocity and random direction.

18, 19, 20], we investigate the diffusion property for the above cases subsequently. For a particle starting at the origin at time  $t = 0$  and diffusing along  $x$  direction, the mean square displacement  $\langle (x(t) - x(0))^2 \rangle$  characterizes its diffusion behavior. For normal diffusion, the Einstein relation of  $\langle (x(t) - x(0))^2 \rangle = Dt$  holds, where  $D$  is diffusion coefficient. If the mean square displacement does not grow linearly in time, i.e.,  $\langle (x(t) - x(0))^2 \rangle = Dt^\beta$ , we refer to anomalous diffusion. Recently, the connection between anomalous diffusion and corresponding heat conduction in 1D system was discussed hotly [18, 19, 20]. We plot the mean square displacement versus time  $t$  in Fig. 4(c) for the aforementioned four cases. Note that  $10^5$  particles were put at the center of the channel where  $x = 0$  with unit velocity and random direction in the simulations. The top solid line and the bottom short-dash-dot line are precisely straight in the whole simula-

tion period ( $t = 10^5$ ), which correspond to the case I (non-chaotic) and case IV (strong chaotic), respectively. We obtain  $\beta = 1.628$  for the case I which corresponds to  $\alpha = 0.721$ , and  $\beta = 1.001$  to  $\alpha = 0.009$  for the case IV. Beyond these two cases do the curves keep asymptotically linear at large time  $t$  with diffusion exponent  $\beta$  between the values of above two cases. The best fits of the slope give  $\beta = 1.357$  which corresponds to  $\alpha = 0.526$  for case II and  $\beta = 1.050$  to  $\alpha = 0.101$  for case III, respectively. The relation between divergent exponent  $\alpha$  and diffusion exponent  $\beta$  fits the relation of  $\alpha = 2 - 2/\beta$  proposed by Li and Wang in Ref. [18], as is plotted in Fig. 4(b). Whereas Denisov *et al.* presented another connection of  $\alpha$  with  $\beta$  on the basis of the Lévy walk model [20]. More details about the origin of the discrepancy between above two relations can be found in Ref. [19].

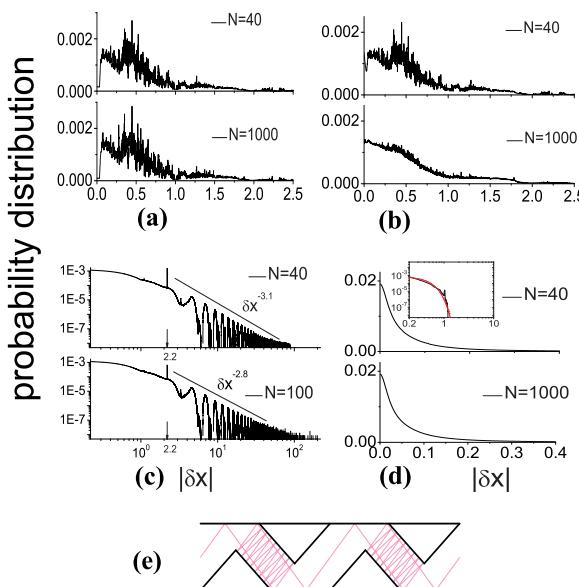


FIG. 5: (color on line) (a), (b), (c) and (d) The PDFs of the flight distance  $|\delta x|$  between two consecutive collisions for above four cases I, II, III and IV respectively.  $N$  represents the system size. Note that the log-log scale is used in (b) and the inset of (d). In the latter case (d), Gaussian distribution (red dashed-line) is in comparison to the numerical PDF. (e) The typical trajectory with periodicity in case of  $R = 0$ ,  $h = 1.0$ .

As different diffusion behaviors are likely related to the trajectory characteristics of the particle propagation, we investigate the PDF  $\psi(|\delta x|)$  of the flight distance  $|\delta x|$  in  $x$ -direction between two consecutive collisions with the scatters. After a long time for adequate collisions in the channel, the PDF for aforementioned fore cases, shown in Fig. 5(a) to (d) respectively, take on completely different forms for different cases. In case I, the discrete values of probability indicate that the trajectories are abundant of periodicity, which is almost alike for larger system size.

The maximum value of PDF appears when  $|\delta x| = 0.447$ , and the typical trajectory is plotted in Fig. 5(e) which shows explicitly that the parallel passage makes the periodical trajectory possible, and the particles are easier to propagate along the channel with fewer collisions. It is superdiffusion in this case. In case II, only smaller system size has the explicit periodicity. With the system size growing, the periodicity is destroyed by the collisions with the segment of circle time and time. The PDF gets smoother in this case. In case III, the periodicity happens only for large flight distance  $|\delta x|$  with very small number of families. Note that the maximum of PDF is corresponding to the value  $|\delta x|$  of 2.2 which is just the length of a cell, and the PDF decays in power law. In this case it requires more collisions and takes more time for the particles to escape a certain region. Thus the propagation is suppressed but is still of superdiffusion. The normal diffusion takes place when the particles are scattered by sufficiently large density of hyperbolic scatters (case IV). Consequently, the strong chaos presents the trajectory of heat carriers with more aperiodicity. The PDF takes on its characteristic form which has a Gaussian tail as shown in the inset of Fig. 5(d).

Thus, the propagation modes are responsible for the diffusion behavior. The abundance of aperiodicity of trajectory is the characteristic of chaotic channel and may also play an crucial role in the normal diffusion. In other words, if the trajectory in a certain system emerges the aperiodicity due to some other mechanisms, such as in polygonal billiard gas model [15], the normal diffusion behaviors may happen.

#### IV. THE CALCULATION OF TEMPERATURE FIELD

We calculate the temperature field following the approach proposed in Ref. [10]. The temperature of  $i$ th cell is defined by averaging the kinetic energy over all visits into the cell

$$T_i = \langle E_i \rangle = \frac{\sum_{j=1}^m t_j E_{ij}}{\sum_{j=1}^m t_j}, \quad (5)$$

where  $t_j$  denotes for the time spent within the cell in the  $j$ th visit, and  $m$  for the total number of visit. For sufficiently large  $m$  we expect a steady temperature profile, and this is indeed verified in our calculations for totally  $10^{10}$  visits. The temperature profiles we obtained are plotted in Fig. 6. It is worthwhile to point out that the steady temperature profiles between non-chaotic and chaotic system are quite different in thermodynamics limit, which is due to the different diffusion behaviors as shown in Fig. 4(c). As case I is non-chaotic and has uniform diffusion exponent  $\beta$ , the temperature profiles

keep almost the similar shape for different system sizes. At the two ends of channel there are large temperature jumps which play an important role in the Fourier transport and dynamics of the system [21]. These jumps arise from the boundary heat resistance which usually appears when there is a heat flux across the interface of the two adjacent materials. In case II and III which are chaotic and have asymptotically decreasing  $\beta$  versus time  $t$ , there also exists the boundary heat resistance. Unlike in case I, the temperature jump here is smaller and diminishes when the system size grows. For larger size is there almost no temperature jump which corresponds to a nearly linear temperature profile. Both the larger system size  $N$  and the arc radius lead to the increase of chaos degree which is responsible for the decrease of diffusion exponent  $\beta$  ( $\geq 1$ ). In case IV, which is strong chaotic, the temperature profiles are almost linear for various system sizes we considered, corresponding to the normal heat conduction.

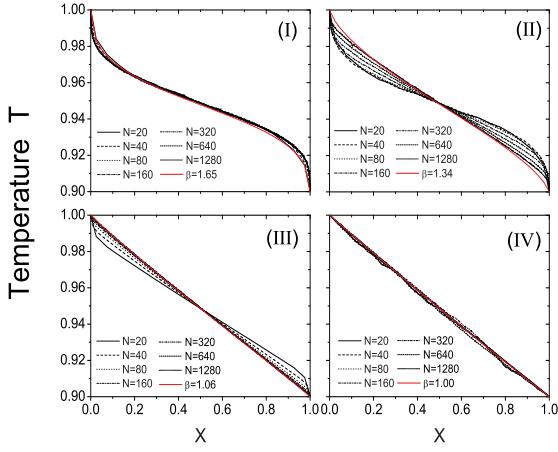


FIG. 6: (color on line) Numerical results of temperature profiles for  $T_L = 1.0$ ,  $T_R = 0.9$  and sizes  $N = 20$ (solid), 40(dash), 80(dot), 160(dash dot), 320(dash dot dot), 640(short dash) and 1280(short dot), respectively. The four panels refer to (I) $R = 0$ ,  $h = 1.0$ ; (II)  $R = 0.001$ ,  $h = 1.0$ ; (III)  $R = 0.848528$ ,  $h = 1.0$ , and (IV)  $R = 0.848528$ ,  $h = 0.27$ . The red lines correspond to the best fits for the numerical temperature profile at  $N = 1280$  with Eq. (8), giving the analytical values  $\beta$  with 1.65, 1.34, 1.06 and 1.00 for above four cases respectively.

We estimate the temperature profiles from the average point of view. Considering the incident particles from the left heat bath (where  $x = 0$ ) propagating along the x-axis to the right end, we suppose that a reflecting boundary is placed at the origin of the x-axis and an absorbing one at the other end. When  $2 \geq \beta \geq 1$ , we assume that the mean density  $n_L(x)$  of the particles at site  $x$  in the steady state is proportional to  $(1 - x)^\gamma$  with  $\gamma = (2/\beta - 1)\beta^{3/2}$ , where we set  $x = i/N$ . Under this assumption, we have

$n_L(x) \sim 1 - x$  [10] when  $\beta = 1$  (normal diffusion) and  $n_L(x) \sim \text{const}$  when  $\beta = 2$  (ballistic diffusion). The conservation of particle number requires

$$n_L(x) \sim \frac{(1 - x)^\gamma}{D_L}, \quad (6)$$

where  $D_L$  are the diffusion coefficient. Likewise, for a particle propagating from right to left, we have

$$n_R(x) \sim \frac{x^\gamma}{D_R}, \quad (7)$$

We assume  $D_L = T_L^{\beta/2}$  and  $D_R = T_R^{\beta/2}$ . Thus, if  $2 \geq \beta \geq 1$ , the temperature is given by

$$\begin{aligned} T(x) &= \frac{T_L n_L(x) + T_R n_R(x)}{n_L(x) + n_R(x)} \\ &= \frac{T_L T_R^{\beta/2} (1 - x)^\gamma + T_L^{\beta/2} T_R x^\gamma}{T_L^{\beta/2} x^\gamma + T_R^{\beta/2} (1 - x)^\gamma}. \end{aligned} \quad (8)$$

where  $\gamma = (2/\beta - 1)\beta^{3/2}$ .

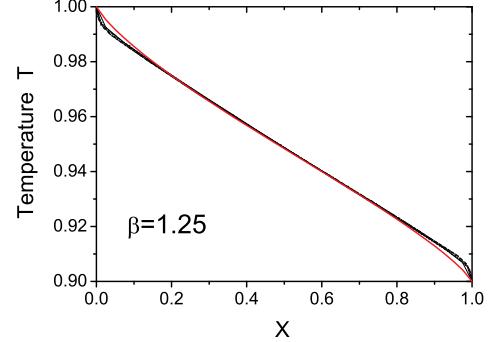


FIG. 7: (color on line) Numerical results of temperature profile in comparison to the analytical results. The numerical temperature profiles with  $R = 0.848528$ ,  $N = 40$ ;  $R = 0.4$ ,  $N = 40$ ;  $R = 0.2$ ,  $N = 40$ ;  $R = 0.1$ ,  $N = 80$ ;  $R = 0.05$ ,  $N = 160$  at  $h = 1.0$  and  $R = 0.848528$ ,  $N = 20$  at  $h = 0.5$  almost share the same shape. The red line is the plot of Eq.(8) with  $\beta = 1.25$ .

As shown in Figs. 6 and 7, the analytical results (in red lines) are in good agreement with the numerical ones for all the cases except those at the two ends of the channel for superdiffusion cases. These deviations are likely due to the different boundary conditions we used. Furthermore, the value of  $\beta$ , obtained by the best fits for the numerical temperature profile at  $N = 1280$  with Eq. (8), agrees with the simulating result greatly for aforementioned four cases. One can see clearly from Eq.(8) that temperature profiles are closely related to the diffusion exponent  $\beta$ , namely, the case with smaller diffusion exponent tends to have smaller temperature jump. Accordingly, it is not unexpected that different chaotic cases may share the

same temperature profile if they have the identical diffusion exponent  $\beta$ . As shown in Fig. 7, the case with smaller diffusion exponent requires smaller system size for achieving the same temperature profile. Moreover, our calculations show that the results of Eq.(8) are consistent with the numerical ones even in larger temperature gradient. Thus, the temperature profile is mostly dependent on the diffusion behavior which is remarkably affected by the finite-size effect for chaotic cases of superdiffusion.

## V. DISCUSSION AND CONCLUSION

In summary, we have investigated the role that the chaos plays in the heat conduction by billiard gas channel. We have demonstrated that the degree of dynamical chaos is enhanced by increasing the arc radius or the system size for chaotic channel, and the mass and heat transport behavior is significantly related to the degree of dynamical chaos of a channel. The stronger the chaos is, the closer to normal transport behaviors the model seems to be. Furthermore, our numerical results of two exponents  $\alpha$  and  $\beta$  for both non-chaotic and chaotic cases when  $\beta \geq 1$  satisfies the formula  $\alpha = 2 - 2/\beta$  [18]. We also discussed the microscopic dynamics by the PDF of flight distance in  $x$ -direction. It seems that aperiodicity of trajectory plays an important role in diffusion behavior. Finally, our results showed that the temperature jumps at both ends of the channel depend mostly on the diffusion property for both non-chaotic and chaotic channels, and the finite-size effect is more crucial for chaotic ones.

As is known that the billiard gas model is applicable for capturing the underlying dynamics of particles without interaction. It is therefore worthwhile to discuss the relation between our work and others in this field.

Alonso *et al.* [10] investigated 1D Lorentz gas model full of periodically distributed half circular scatters. By defining the heat conductivity and temperature field as statistical average over time on the hypothesis of local thermal equilibrium, the Fourier law holds in this case, and a linear gradient is given for quite small temperature difference. Our work starts from the same approach but different scatter geometry is taken into account. Thus it is not surprising that our work has some overlap with theirs in spirit. However, we pay much more attention to the role played by different degree of dynamical chaos in heat conduction. As a result, our intensive calculations extended the results in Ref. [10] and concluded that only sufficient strong chaos results in the normal diffusion, thus, the normal heat transport.

Li *et al.* [14] presented the dependence of heat conductivity on system size and the temperature profile in channel with zero Lyapunov exponent where the right triangle scatters are periodically distributed. In this case, the exponent stability leads to abnormal transport behavior. Clearly, their result is the non-chaotic limit of our model.

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